(E)-Nuciferol isobutyrate

Inchi: InChI=1S/C18H26O2/c1-13(2)18(19)20-16(5)8-6-7-15(4)17-11-9-14(3)10-12-17/h8-13,15
InchiKey: HPZWBNSNFMOEME-LZYBPNLTSA-N
Formula: C18H26O2
SMILES: CC(=CCCC(C)c1ccc(C)cc1)OC(=O)C(C)C
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	36.33	kJ/mol	Joback Method
hf	-337.72	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.982		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2004.00		NIST Webbook
tb	722.35	K	Joback Method
tc	930.19	K	Joback Method
tf	354.68	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.06	J/mol×K	722.35	Joback Method
cpg	706.05	J/mol×K	756.99	Joback Method
cpg	722.94	J/mol×K	791.63	Joback Method
cpg	738.79	J/mol×K	826.27	Joback Method
cpg	753.64	J/mol×K	860.91	Joback Method
cpg	767.53	J/mol×K	895.55	Joback Method
cpg	780.52	J/mol×K	930.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume